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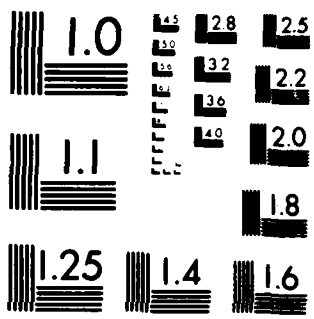

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INVESTIGATIONS OF THE INTERACTIONS OF RADIATION WITH MATTER

FINAL REPORT

STEVEN T. MANSON

MAY 31, 1983

U. S. ARMY RESEARCH OFFICE

DAAG29 80 C 0027

GEORGIA STATE UNIVERSITY

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REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER / 2. GOVT ACCESSION NO. A129980	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Investigations of the Interactions of Radiation with Matter	5. TYPE OF REPORT & PERIOD COVERED Final Report Jan 1980 - Feb 1983
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Steven T. Manson	8. CONTRACT OR GRANT NUMBER(s) DAAG29 80 c 0027
9. PERFORMING ORGANIZATION NAME AND ADDRESS Georgia State University Atlanta, Georgia 30303	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office Post Office Box 12211 Research Triangle Park, NC 27709	12. REPORT DATE 31 May 1983
	13. NUMBER OF PAGES 9
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report) Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA

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18. SUPPLEMENTARY NOTES

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Photoionization photoabsorpiton, ionization, relativistic effects, inelastic collisions, excited states, x-rays, inner shells, ions, cross sections

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Work on the interaction of radiation with matter is described. In particular photoabsorption by ions and excited states is discussed, along with relativistic effects in the photabsorption by heavy elements and charged particle impact ionization of atoms. The relevance of these areas to various applied areas such as radiation protection and safety, x-ray laser schemes and effects, nuclear pumped lasers, and IR detection is pointed out.

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Over the period of this grant from the U.S. Army Research Office, we have been actively engaged in research into theoretical atomic and ionic physics. In what follows the major areas of our investigations shall be discussed, along with the progress that has been made in those areas. In addition, we shall also discuss, where applicable, the relevance of the research findings to various Army needs in the area. The discussions are as non-technical as possible, but ample references are given to published works where the technical details can be found.

I. Photoabsorption by Excited States

Excited states of atoms are produced in quantity in hot environments, such as in the vicinity of an atmospheric thermonuclear blast; thus their properties are of interest. In addition, a detector in the IR range, with a quantum efficiency of unity, is now possible using lasers to excite atoms to states with ionization potentials in the IR range. Therefore, photoabsorption cross section for excited atomic states are required.

In our studies several important features of excited state photoabsorption have emerged.[1-3] First is that the cross sections can be extremely large, at threshold, and they increase with increasing principal quantum number n. Next is that the cross sections fall off extremely rapidly from threshold, faster with increasing n and angular momentum ℓ. These characteristics of the photoabsorption allow for the possibility of IR detectors at different wavelengths with the further possibility of various band widths in a given wavelength range.

Our studies have also found multiple minima in the cross sections of certain types of excited states. Some of these minima lead to dramatic absorption windows for certain wavelengths. In Cs, for example, the excited 5d state is predicted

to have such a window[4] and the excited 9d states is predicted to have two such windows.[3] In addition certain less dramatic minima have been found[1-4] which do not exist for ground states.

II. Photoabsorption by Positive Ions

Positive ions are also produced in any very hot environment, as discussed above. Their properties are, therefore, of interest in this connection as well as in connection with the passage of a possible x-ray laser beam through the atmosphere.

We have completed our studies of the photoabsorption of positive ions. Previously we had uncovered the systematics of the process for low - and medium - Z atoms.[5-6] We have now done a high - Z case[7] (Z=80, Hg) and found that the systematics remain the same. Inner shell cross sections remain constant, apart from a shift of threshold, when outer electrons are removed. It is also found that various features of the cross section such as Cooper minima[8] or delayed maxima,[9] hardly move even when electrons from the same shell are removed. This knowledge is extremely useful as it allows the prediction of the properties of ionic photoabsorption from the characteristics of photoabsorption by neutral atoms.

III. Relativistic effects in Photoabsorption by Heavy Elements

Photoabsorption by heavy elements in the UV and x-ray range is or importance in the area of radiation physics generally, and specifically in the areas of radiation protection and shielding of personnel and materials. While the situation is fairly well-understood for light elements, for heavy elements the situation is otherwise.

We have embarked upon a study of photoionization cross sections for high-Z atoms. This theoretical study was performed within the framework of the explicitly relativistic Dirac equation so as to incorporate the relativistic interactions a priori and not as perturbations.

A major focus of this study has been the relativistic effects on Cooper minima[8] in the photoionization cross section. These minima, pervasive in $\ell \rightarrow \ell + 1$ transitions in outer and near-outer subshells throughout the periodic system,[10] are caused by quantum mechanical interference effects. Relativistic interactions split a single non-relativistic minimum into three distinct minima (two for photoionization of s-states). It was expected that the energy separation (splitting) of these relativistic minima should be the same order of magnitude as the spin-orbit splitting of the energy levels in the ground states. In fact we find splittings more than an order of magnitude larger![11] These splittings give cross sections for spin-orbit doublets which differ appreciably. This may have an important analytical application to the very heavy elements such as radium, radon, uranium, and plutonium.

In addition, these minima have profound effects on the photoelectron angular distributions which are of importance in radiation transport and the disposition of energy in biological tissue.

We have also studied the overall systematics of the cross sections of a number of subshells,[12,13] as a function of atomic number, with an eye to ascertaining the utility of simpler non-relativistic methodologies in photoionization of heavy elements. Our results so far show significant deviations in certain cases owing to relativistic interactions, indicating that non-relativistic calculations should be viewed with great caution in this range.

Unfortunately, there is little in the way of experiment to give us a guide as to the accuracy of our results. The little there is Hg 5d, for example, gives excellent agreement with our calculations![14] We are, in any case, continuing this work, to provide a coherent picture of the systematics of photoabsorption by heavy atoms.

IV. Charged Particle Impact Ionization of Atoms

The range and energy loss of charged particles passing through matter is almost solely related to the energy loss via ionization of the matter

by the charged particles. Thus a knowledge of these cross section is the main constituent of calculations of radiation protection and shielding of both men and materials.

Another important application is for the possibility of nuclear-pumped lasers, i.e., dealing with the energy transfer of energetic fission fragments to a (hopefully) lasing medium. Ionization cross sections of the medium materials, along with the spectrum of secondary electrons which cause further ionizations and excitations, are of crucial importance in modelling the nuclear-pumped laser situation.[15]

In still another situation, that of the passage of an ion or neutral particle beam through the atmosphere or other media, the limiting factor of its penetration is the cross section for inelastic collisions, which are mostly ionization.

Finally, ionization cross sections of atoms by charged particle impact is of importance in the possibility of creating population inversions which are useful in deducing possible schemes for an x-ray laser. Thus these cross sections, which are of interest for all three of the above applications, are needed. Many of them are either unobtainable experimentally (at the present level of technology) or simply unavailable. Thus, the need for theoretical estimates is great.

Our work has dealt with total cross sections, single differential cross sections (SDCS) or energy distribution of secondary electrons, and double differential cross sections (DDCS) or energy and angular distribution of secondary electrons. The total and SDCS are the primary results needed as input for the applied areas, but the DDCS is necessary to elucidate ionization mechanisms and to fully assess the validity of the calculational work.

Our major work, in this area, has been on ion-atom collisions where the incident ion brings in its own electrons; previous work had dealt with bare incident particles.[16] We chose as a prototype system $He^+ + He$ for simplicity.[17,18] Our calculated DDCS showed very good agreement with experiment indicating that we have included all of the major mechanisms for electron emission. Note that this includes emission from both the target and the projectile. Unfortunately, no experimental work has yet been done which measures the electrons from projectile and target separately, but the total, as mentioned above, does show good agreement between experiment and our calculation. We are presently engaged in extending this work in two directions. First to more complex collision pairs which are relevant to various areas, and second to neutral-neutral collisions. For both of these extensions, we can use the technology (computer codes) developed for the $He^+ + He$ work.

In related work, we have considered electron impact ionization of inner shells related to electron microscopy.[19] The problem arises from using an electron microscope in the energy loss mode for analytic purposes. The shape of the transmission function differs from that of the ionization cross section in that an electron microscope scans a limited angular range which depends upon the electron energy and the characteristics of the particular instrument. We have performed calculations which provide generalized oscillator strengths which can be easily used by individual microscopists to generate the data for his or her particular instrument.

In the course of this work, we found that interesting edge structures occur even for very inner shells,[20,21] e.g., the K-shell. Previously it had been expected that K-shell energy-loss cross sections maximized at threshold and fell off monotonically with increasing energy loss. This is <u>not</u> the case and structures have been found in most elements above Z = 10. Not only edge structures have been found, but also modulations of the cross section are in evidence. These

modulations extend out some several hundred e V above threshold and are basically caused by atomic interference effects.[20,21] These edge shapes and modulations are useful as analytical tools. More importantly, a similar phenomenon in solids, known as EXAFS (extended x-ray absorption fine structure) is widely used to obtain structural information on solids. These atomic EXAFS, which we have found, could well be confused with the solid EXAFS making the structural information obtained not unambiguous. The study of these structures is continuing.

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January, 1980 - February, 1983

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